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Fluid flow processes at basin scale

Procesos de circulación de fluidos a escala de cuenca

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ABSTRACT

Subsurface fluid flow plays a significant role in many geologic processes and is increasingly being studied in the scale of sedimentary basins and geologic time perspective. Many economic resources such as petroleum and mineral deposits are products of basin scale fluid flow operating over large periods of time. Such ancient flow systems can be studied through analysis of diagenetic alterations and fluid inclusions to constrain physical and chemical conditions of fluids and rocks during their paleohydrogeologic evolution. Basin simulation models are useful to complement the paleohydrogeologic record preserved in the rocks and to derive conceptual models on hydraulic basin evolution and generation of economic resources. Different types of fluid flow regimes may evolve during basin evolution. The most important with respect to flow rates and capacity for transport of solutes and thermal energy is gravitational fluid flow driven by the topographic configuration of a basin. Such flow systems require the basin to be elevated above sea level. Consolidational fluid flow is the principal fluid migration process in basins below sea level, caused by loading of compressible rocks. Flow rates of such systems are several orders of magnitude below topography driven flow. However, consolidation may create significant fluid overpressure. Episodic dewatering of overpressured compartments may cause sudden fluid release with elevated flow velocities and may cause a transient local thermal and chemical disequilibrium between fluid and rock. This paper gives an overview on subsurface fluid flow processes at basin scale and presents examples related to the Penedès basin in the central Catalan continental margin including the offshore Barcelona half-graben and the compressive South-Pyrenean basin.

Keywords: Fluid flow. Paleohydrogeology. Sedimentary basins. Episodic flow. Preferential pathways. Modelling.

RESUMEN

El flujo de fluidos en el interior de la corteza terrestre juega un papel importante en muchos procesos geológicos, lo que ha llevado recientemente a un importante incremento de los estudios sobre la evolución del flujo de fluidos a escala de las cuencas sedimentarias.

Las reservas económicas, tales como petróleo o depósitos minerales, se interpretan como el resultado del flujo de fluidos a escala de cuenca durante largos periodos de tiempo. Los sistemas de flujo fósiles pueden estudiarse mediante el análisis de las alteraciones diagenéticas, de las inclusiones fluidas y de los cementos. Este análisis permite conocer las condiciones físicas y químicas de los fluidos y de las rocas durante su evolución paleohidrogeológica. Los modelos de simulación a escala de cuenca son utilizados para complementar el registro preservado en las rocas y para desarrollar modelos conceptuales de la evolución hidráulica de la cuenca y de la generación de las reservas económicas. Durante la evolución de una cuenca, el régimen de flujo puede evolucionar de un tipo a otro. El régimen más importante, en lo que se refiere a velocidad y capacidad de transportar solutos y energía térmica, es el flujo gravitacional originado por la topografía, cuyo principal requisito es que existan zonas de la cuenca, o alrededor de ella, con elevaciones por encima del nivel del mar. Cuando no existe esta condición, el principal régimen de migración de fluidos es el flujo por consolidación. Las velocidades de flujo originadas por este mecanismo son varios órdenes de magnitud inferiores al flujo originado por la topografía, pero a pesar de ello es capaz de crear sobrepresiones importantes. La pérdida episódica y repentina de agua en estos compartimentos sometidod a sobrepresión suele realizarse a velocidad elevada, lo que origina desequilibrios térmicos y químicos, temporales y locales, entre el fluido y la roca.

El trabajo que se presenta a continuación es una síntesis de los procesos de flujo de fluido en el interior de la corteza terrestre a escala de cuenca y muestra los ejemplos de las cuencas distensivas de los semi-grabens del Penedès y del offshore de Barcelona, y de la cuenca compresiva sur-pirenaica.

Palabras clave: Flujo de fluidos. Paleohidrogeología. Cuencas sedimentarias. Flujo episódico. Conductos preferenciales. Modelización.

INTRODUCTION

Sedimentary basins are sediment-filled depressions in the upper crust which preserve sufficient permeability to permit flow of fluids. Many basins accommodate important mineral and energy resources, which have been generated due to fluid flow and fluid interaction with rocks. Sedimentary basins are therefore increasingly being studied in terms of large scale hydrogeologic systems acting over long time spans. The focus of such studies is to characterize the main hydrostratigraphic units, to reconstruct the paleohydrogeological evolution and to determine the hydrogeochemical evolution of fluids within the basin fill. Key information for the paleohydrogeological reconstruction is preserved in the diagenetic evolution of sedimentary deposits and in the composition of fluid inclusions in the cements formed in pores and fractures. Therefore, paleohydrogeologic reconstruction requires to consider the sedimentologic, tectonic, thermal and hydrogeochemical processes. These processes constitute components of a complex feedback system, which transfers and redistributes mass and thermal energy within a sedimentary basin. Depending on the type of sedimentary basin, the geometry, facies evolution and stratigraphic architecture vary through time, and different hydrogeologic regimes may contribute to the transfer of mass and energy. As basins subside, sediments and fluids are buried and heated up due to heat conduction from the earth's interior and partly by heat production in the crust from radioactive decay. Thus, fluids and rocks experience changing physical and chemical conditions during sedimentary basin evolution, leaving fingerprints in the rocks which can be identified as a series of superimposed diagenetic alterations. Unfortunately, the paleohydrogeologic record in rocks is not preserved as a series of datable and unequivocal products. Instead, the record is usually an incomplete set of uncertain information, similar to the stratigraphic record preserved in a sedimentary column, which does not represent a continuous array of time. With increasing timespan represented in a sedimentary column, the hypothesis which becomes more probable is that the stratigraphic information preserved therein is incomplete. Similar to erosional events which reduce stratigraphic completeness of a sedimentary column, fluid-rock interaction such as mineral dissolution reduces the completeness of the paleohydrogeologic record. In addition, diagenetic reactions are not always unequivocally linked to the corresponding flow process and not every hydrogeologic stage leaves a detectable fingerprint in every part of the deposit. Mineral precipitation or dissolution can occur without any fluid flow taking place if temperature or pressure conditions in the rocks change through time.

Changes in physical and chemical conditions during basin evolution control the interaction between pore fluids and rocks. Sedimentary rocks consolidate and may be cemented or dissolved, thereby changing their chemistry, texture and ability to transmit fluids, solutes and heat. At the same time, fluids change their hydrochemical composition and may become more diluted or more concentrated. As these fluids change in temperature, they may dissolve minerals, which later occasionally precipitate as ores when mixed with other fluids or if a further change of temperature occurs. Hydrocarbons generated by organic matter rich sediments may be transported towards reservoir rocks, if physico-chemical conditions and timing are appropriate. Flow, transport and reaction in the scale of sedimentary basins are in most cases slow and steady processes. However, over the scale of geologic time, its effects are of great importance as they can generate important resources. The study of fluid flow and the interaction between fluids and rocks has considerably advanced due to progress both in simulation techniques and analytical methods. Paleohydrogeologic simulation permits to represent flow processes in a simplified way and to test hypotheses, to derive conceptual models of fluid flow in basins and to make predictions based on geological data of a particular sedimentary basin. An introduction to mathematical fundamentals of such models is given by Person et al. (1996).

CHARACTERISTICS OF BASIN FLUIDS

With respect to the origin of basin fluids, Lawrence and Cornford (1995) distinguish between internally derived fluids such as formation waters (connate waters) and hydrocarbons, and externally derived fluids such as meteoric and metamorphic fluids. Another internal source of fluid is related to clay diagenesis, which may contribute to overpressure build-up in subsiding basins (Bethke, 1986). However, diagenetically released fluid mass is probably small compared to fluids released by mechanical sediment compaction. To minor degree, water from the underlying basement also contributes to basin fluids. The different fluids can be detected through their individual geochemical signature; however, the signal of individual fluid components may be weak depending on mixing processes. Initial fluid content evolves geochemically due to reactions with adjacent rocks and mix at least partially with externally derived fluids. As a result, most basins contain mixtures of different types of fluids, depending on the evolution of basin hydrology.

Most sediments initially contain pore fluids which correspond to meteoric fluids or marine fluids depending on the subaquatic environment at the time of deposition. This connate water is buried with the sediment and can be identified through its chemical properties. In case of nonmarine sedimentation, initial fluids are derived from meteoric waters that enter the earth's crust as rainfall. Its chemical signature (trace elements and isotopes) allows to draw conclusions on the topography and climatic situation of the recharge area. In case of marine deposition, initial fluids are seawater and its chemical signature allows to draw conclusions on salinity and degree of evaporation.

Mixing of different waters in sedimentary basins appears to be a principal process which controls the hydrochemical evolution of basin fluids. Such mixing is evident in the Br-Cl systematics of waters in many sedimentary basins, which can only be accounted for by mixing of various end-member water types (Hanor, 1994). Sodium chloride is the principal salt in brines. As chloride anions do not interact in mineral formation or diagenetic processes, chloride is considered to be a conservative tracer. The distribution of salinity in sedimentary basins reveals therefore important information to constrain paleohydrogeological basin evolution. The observation of brines at considerable distance from evaporites is a strong argument for the existence of large scale fluid flow taking place in many basins (Bjørlykke and Gran, 1994).

Changes of chemical pore fluid composition due to fluid rock interaction are controlled by temperature, pressure and chemical composition of the adjacent rocks. If flow is slow, fluids will chemically equilibrate with the surrounding rocks and may cause dissolution or precipitation of minerals. Reactions between fluids and rocks are evident in the observation that solute content of fluids increases with burial depth and age. The concentration increase is sometimes almost linear with depth, if evaporites are located at the base of a sedimentary sequence (Dickey, 1979). At depth, basin fluids become high-density brines with elevated halite concentrations. Such fluids are frequently associated with hydrocarbon fluids (Carpenter, 1978).

Geochemical data indicate that brines are in most cases derived from evaporite pore fluids and from fluid interaction with enclosing sedimentary rocks. Salinity gradients of North Sea formation waters show a clear coincidence with the presence of evaporites in the basin. Based on this observation, Bjørlykke and Gran (1994) suggest that most brines are derived from meteoric water interacting with salt formations. Gravitational settling of ions has been discarded as a possible source of brines. Ultrafiltration through shales acting as semipermeable membranes is capable of changing solute concentration and might account for some of the increasing salinity with depth (Neglia, 1978), however, the importance of this process remains uncertain. On the other hand, experiments have shown that ultrafiltration through low permeable shales affects the isotopic composition (Coplen and Hanshaw, 1973).

HYDRAULIC PROPERTIES OF SEDIMENTARY BASINS

Large-scale fluid migration is caused by gravitational flow due to infiltration of meteoric fluids in topographically elevated areas and fluid discharge in areas of lower topographic elevation. Another process creating hydraulic gradients is the consolidation of the sediment. To a lesser extent, thermal convection also may contribute to fluid flow. Dissipation of hydraulic gradients and the corresponding fluid flow are controlled by the hydraulic properties of the basin fill. The main controlling rock properties are hydraulic conductivity and the specific storage. Porosity and curvature of the flow path within the pores as expressed by the tortuosity of the pores play significant roles in solute transport. Hydraulic conductivity as well as specific storage are closely linked to porosity (see Appendix).

Heterogeneity

At the scale of sedimentary basins, the heterogeneity of rocks is a controlling factor for the distribution of fluid pressure and flow rates. Heterogeneity is primarily created from the sedimentation process, which provides a more or less complex distribution of sedimentary facies determined by various geological conditions. As a result, hydraulic properties in a sedimentary basin are heterogeneously distributed with high permeable/low compressible materials at the basin margins and low permeable/high compressible materials in the basin centre, as a general rule. Heterogeneity is a scale dependent property. At a microscopic scale only pores and grains exist with an elevated degree of heterogeneity. At a larger scale the statistical distribution of individual pore geometries and pore connectivity permits to consider the rock as a homogeneous porous medium with hydraulic properties representing a statistical average of the considered rock volume. Thus, heterogeneity needs to refer to an observational scale. This effect is commonly acknowledged in analysing dispersive solute transport and needs to be taken into account for hydraulic conductivity as well.

Anisotropy

Anisotropy of hydraulic properties such as hydraulic conductivity implies that such properties have different magnitude with respect to the orientation of flow within a rock volume. This is mainly caused by the geometry and connectivity of the pore space. Pore connectivity is usually elevated in the bed plane, and hydraulic conductivities may be considerably elevated in the bed plane. Whereas coarse grained, well sorted and well rounded sediments tend to have a low anisotropy, fine grained sediments may exhibit important anisotropy due to the microscopic parallel arrangement of clay aggregates. Anisotropy is often related to the sedimentation process that created the deposit. In case of hydraulic conductivity, the main direction imposed by the sedimentation process often determines the direction of maximum hydraulic conductivity. For instance, carbonate reefs may have increased hydraulic conductivity in the vertical direction, and reefs may therefore act as vents for pore water (Chapman, 1987). Fractures, cleavage and fault systems can also provide anisotropy. Variograms have been successfully applied as a measure of spatial variability of hydraulic parameters (deMarsily, 1986).

Hydrostratigraphic units

In order to facilitate the paleohydrogeological reconstruction of a sedimentary basin, the basin fill is usually divided into hydrostratigraphic units. These units are defined by their hydraulic properties such as hydraulic conductivity, compressibility, grade of heterogeneity, anisotropy and degree of lateral continuity. Some of these properties vary through geologic time, as for example consolidation reduces pore space, elastic properties and hydraulic conductivity. Fracturing due to tectonic processes may also create important changes in hydraulic properties during basin evolution. Such changes of hydraulic properties make definition of hydrostratigraphic units a difficult task in paleohydrogeologic modelling. The purpose of distinguishing hydrostratigraphic units is to represent hydraulically similar responding rock units within a hydrogeologic model. Model discretization should therefore take into account the definition of hydrostratigraphic units.

FLUID MOVING PROCESSES

Three principal processes causing fluid flow at basin scale are discussed here: topography driven fluid flow, consolidational fluid flow and thermal convection.

Topography driven fluid flow

Gravitational flow due to topographic gradients is the most important fluid migration process in a basin. Meteoric fluids enter a sedimentary basin through rainfall and flow as groundwater at shallow depth in local or regional aquifers. However, depending on the hydrostratigraphic configuration of the basin, meteoric fluids also migrate into deeper units of the basin. Fluid discharge is usually located at low topographic elevations, where fluids migrating through the basin return to surface flow systems such as rivers and lakes. Two conditions must be satisfied to allow topography driven flow: 1) the basin needs at least to be partially elevated above sea level, and 2) the flow system requires recharge by meteoric waters. These conditions can be fulfilled in compressive settings as well as in distensive settings. The persistence and intensity of topography driven flow systems is largely controlled by geographic and climatic conditions.

Changes in topographic elevation due to erosion or tectonic processes also affect evolution of flow systems at basin scale. Uplift may cause underpressure in large portions of a basin if a regional aquifer exists at depth which discharges at a low topographic elevation. Such underpressuring occurs in the north-alpine foreland basin, where jurassic carbonates provide a deep regional aquifer which discharges towards the Danube river. The overlying hydrostratigraphic units of the foreland basin discharge into the regional aquifer (Lemcke and Tunn, 1956), thus presenting a situation of underpressuring, whereas the overthrusted zones of the foreland still exhibit residual overpressures due to previous tectonic loading, involving a consolidation related fluid expulsion. A similar situation of underpressuring is observed in the Southwest Alberta basin (Bachu and Underschultz, 1995).

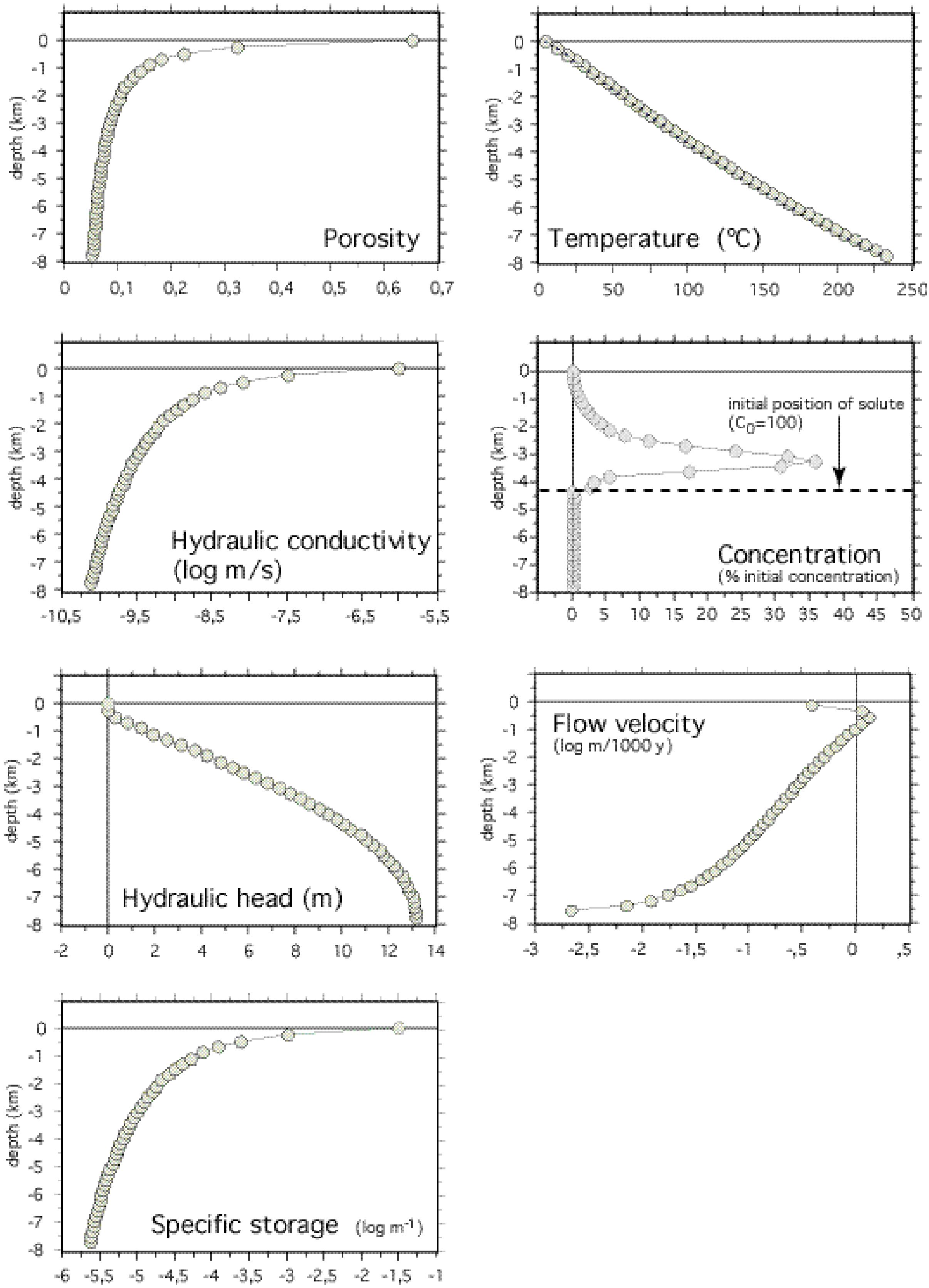
Sea level falls can initiate topography driven fluid flow by exposing parts of a basin above sea level. In this case, topography driven flow takes place in parts of the basin which were previously submerged below sea level. An important consequence of sea level changes is that meteoric water may intrude into deeper parts of a sedimentary basin and cause fluid mixing and diagenetic reactions (Bethke et al., 1988; Bitzer, 1999). The Messinian sea level fall in the Mediterranean may have caused such a flushing of aquifers at depth with important consequences for generation of hydrocarbon reservoirs.

Solute and heat tr anspor t

The capacity to transport solutes and heat by topography driven flow is only limited by the extent of meteoric fluid recharge and the persistence of such flow systems. Infiltrating meteoric fluids have an initially low solute content and low temperature. As they infiltrate into deeper parts of a basin, fluid temperature equilibrates with adjacent rock temperature. This results in an increase of fluid temperature and decrease of rock temperature. Towards the discharge area, fluids ascend and cool down. Correspondingly, a thermal anomaly is caused in the rocks by the redistribution of thermal energy from descending or ascending fluids. Bodri and Rybach (1998) analysed heat flow in a topography-driven flow system in the Swiss Alps and demonstrated that heat flow in fluid discharge zones in valley bottoms is elevated by a factor up to 1.8. Correspondingly, heat flow in the recharge zones is reduced. At a larger scale, the redistribution of fluids bears important consequences on the formation of ore deposits as well as energy resources. In a theoretical study, Gayer et al. (1998) demonstrated that transport of thermal energy due to topography driven flow took place after the climax of the Variscan orogeny. The assumed configuration of the flow system causes the observed asymmetric distribution of coal rank in the South Wales foreland basin with elevated coal ranks at the presumed discharge location of the flow system.

Thermal springs are frequently related to topography driven flow systems. In many cases tectonic structures play an important role through the creation of preferential pathways such as fractures or faults. Tectonic activity may also initiate topography driven flow due to tectonic subsidence or uplift of parts of a basin. As shown by Fernández and Banda (1990) for the Neogene Vallès-Penedès graben in Catalonia, elevated heat flow is not necessarily related to increased internal heat production through magmatic processes or otherwise release of crustal hot fluids. Here, the bounding faults provide a flow channelling and serve as preferential pathways for deeply infiltrating meteoric water from adjacent horsts. Local discharge of such fluids cause elevated heat flow rates at the graben boundaries. Flow and heat redistribution can exhibit complex patterns depending on the heterogeneity of the basin fill, location of conducting layers, preferential pathways and its topographic configuration as shown by Clauser (1989) for the Rhine graben. There, meteoric fluids from the eastern horst block of the graben redistribute heat along basal regional aquifers towards the western part of the basin, where elevated thermal gradients occur due to fluid flow and advective transport along hydraulic conducting faults.

Solute concentration tends to increase with depth, and mineralization can occasionally take place from the cooling of such fluids towards discharge areas (Garven, 1995). Warm brines have moved over hundreds of kilo-



depth (km)
Porosity
Temperature (ºC)
Hydraulic conductivity
(log m/s)
initial position of solute
(C_0=100)
Concentration
(% initial concentration)
Hydraulic head (m)
Flow velocity
(log m/1000 y)
Specific storage (log m^{-1})

metres in the North American continent, generating barium, zinc and lead mineralizations of the Mississippi valley type (MVT). These ores are thought to have formed from brines at temperatures between 75º and 150ºC (Bethke et al., 1988). Heat transport required to generate these deposits is most likely to be caused by topography driven flow created by tectonic uplifting. Deming and Nunn (1991) pointed out that topography driven flow may also be efficient for transporting solutes through the basin, however the flow system is bound to a flushing of the basin, as brines are replaced by cool meteoric waters with low solute concentrations. Deming and Nunn (1991) conclude that the necessity of elevated heat flow by topography driven advection and the presence of brines are incompatible. The origin of hot brines that have formed MVT deposits is therefore difficult to explain with topography driven flow exclusively. Flow rates required to create elevated heat flow at the basin edges flush at the same time the solutes out of the basin, even if a solute source is assumed within the rock.

Petroleum resources are also affected by topography driven flow. Such flow systems can be detected in the inclination of the contact zone between oil and formation waters in reservoirs. Hydrocarbons may be forced by topography driven flow to migrate towards hydraulic traps. However, a frequent result of topography driven flow is the flushing of hydrocarbon reservoirs or the biodegradation of hydrocarbons under the influence of meteoric waters, as for example observed in the northern Alpine foreland basin (Lemcke and Tunn, 1956).

Consolidational f low

Compaction or consolidation related fluid flow is several orders of magnitude less important than topography driven flow with respect to flow velocities and transport capacity. The principal difference to topography driven flow is the absence of an external fluid recharge, causing a closed system. While the amount of fluids involved in topography driven flow is only limited by the amount of meteoric recharge, fluid transport due to sediment consolidation is determined by the amount of fluid that is initially contained within the pores. Transport capacity is therefore low compared to topography driven flow. Consolidation driven fluid flow is induced by loading of compressible and hydraulic conducting rocks due to continued sedimentation or tectonic processes and results in the expulsion of interstitial pore fluids. As this process requires continued loading, it is restricted to the subsidence and filling stage of a sedimentary basin. In compressive sedimentary basins, thrust sheet emplacement may move tectonic brines from deeper parts of the thrusted sedimentary pile along conductive faults (Oliver, 1986). In this case the load of thrust sheets and the lateral compression of the basin cause a fluid expulsion which is essentially a consolidational flow (Bitzer et al., 1998).

As shown by Einsele (1977) and Bonham (1980), mass flux and velocity of consolidational fluid flow systems is limited, as long as no flow channelling along preferential pathways occurs. Maximum consolidational flow velocities are usually less than or in the order of the sedimentation rate. Therefore, advective transport is low and diffusive transport plays a major role. As consolidational flow is related to the basin filling, it is capable of moving solutes at early stages of basin evolution, as has been reported in the South Pyrenean Ainsa basin (Travé et al., 1997). In the absence of topography driven flow, sediment consolidation generates a more or less vertical fluid transfer through the consolidating sediment pile. In case of subaerial deposition and sufficient topographic gradients, consolidational flow will interfere with topography driven flow, and topography driven flow events will usually result in freshwater flushing in some parts of the basin (Wilson et al., 1999, Bitzer, 1999).

Reduction of lithostatic load due to erosion of a low permeable sediment pile may create an elastic dilatation of rock-pore volumes and cause underpressuring. A recent example has been reported from mesozoic shales from the Wellenberg site at Lake Lucerne in Switzerland,

Figure 1. Consolidational fluid flow in a growing sediment column. Sedimentation rate 1m/1000 y, initial porosity 65%, initial hydraulic conductivity 10^{-6} m/s, initial specific storage $10^{-1.5}$ m^{-1}, basal heatflow 1.5 hfu, initial concentration of layer at 4 km: 100, longitudinal dispersivity 400 m, diffusion coefficient 10^{-10} m^2/s.

Figura 1. Flujo por consolidación en una columna creciente de sedimento. La velocidad de sedimentación es de 1 m/1,000 años, la porosidad inicial es de 65%, la conductividad hidráulica inicial es de 10^{-6} m/s, el almacenamiento específico inicial es de $10^{-1.5}$ m^{-1}, el flujo de calor basal es de 1.5 hfu, la concentración inicial en la capa situada a 4 km es de 100, la dispersividad longitudinal 400 m y 10^{-10} m^2/s el coeficiente de difusión.

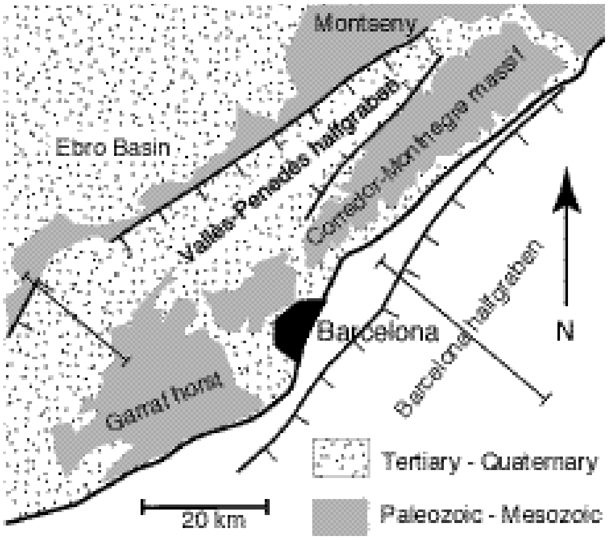


Figure 2. Map of the central part of the Catalan continental margin with location of the simulated cross sections analysed (Figs. 3 and 4).

Figura 2. Esquema geológico del sector central del margen continental catalán con la situación de los dos cortes geológicos modelizados que se muestran en las figuras 3 y 4.

where fluid underpressuring in rocks may be related to a rapid load reduction by glacier melting (Gautschi, pers. communication). Corbet and Bethke (1992) and Parks and Tóth (1995) give examples of underpressuring in low permeable rocks in sedimentary basins due to erosional decompression of rocks.

Because of the limited transport capacity of consolidation driven flow, mineral resources are usually not related to this type of flow. However, sediment compaction has been suggested as a contributing agent for secondary oil migration. Consolidation driven flow can explain only local features involving limited fluid volumes and cannot explain commonly occurring diagenetic features (Bjørlykke and Gran, 1994).

One-dimensional consolidation

A numerical experiment demonstrating the effects of consolidational fluid flow and its capacity to transport solutes and heat is shown in figure 1. In this one-dimensional numerical simulation, consolidation of a compacting sedimentary sequence is calculated, coupling deformation and related fluid expulsion. This is achieved by coupling the consolidation equation with the nonlinear form of the equation of state for porosity (DeMarsily, 1986) and by taking into account the change of hydraulic properties during consolidation (Bitzer, 1996, 1999) using the Kozeny-Carman equation (eq. 7 in Appendix). The sample experiment assumes a growing column of sediment with an initial porosity of 65%, an initial hydraulic conductivity of 10^{-6} m/s, an initial specific storage of $10^{-1.5}$ m^{-1} and a sedimentation rate of 1m/1,000y. The simulation covers a timespan of 20 My. In order to demonstrate the solute transport capacity of consolidational flow, a hypothetic conservative tracer is placed in the initial pore fluid of a layer deposited at 10 My. Figure 1 shows that the sedimentary column reaches a length of about 8 km after 20 My with minimum porosities at the base approaching 5%. Hydraulic conductivities and specific storage decrease with progressing consolidation. Hydraulic head corresponds to fluid overpressure. The low values indicate that the sediment column has almost reached compaction equilibrium. Distribution of flow velocities show values approaching zero towards the base of the column, and maximum values of about 1 m/1,000 y in the upper part of the column, with negligible numerical error due to the moving boundary and the numerical time stepping scheme. This value corresponds well with the sedimentation rate and confirms the conclusion derived by Einsele (1977) and Bonham (1980), that fluid flow in the upper part of a compacting sediment column may approximate the sedimentation rate, if the column is sufficiently thick. The temperature distribution in the column for advective transport and for heat conduction are almost identical, which reflects the predominance of conductive heat transfer over advection. Heat advection from consolidational fluid flow increases slightly temperatures at the base of the consolidating column in the order of a few degrees C. Solute transport, however, shows a more pronounced impact of advection related to consolidational fluid flow. Solutes are transported upward in the order of several hundreds of meters. Fluids in a compacting sediment column must therefore be seen as mixtures of fluids which have been expelled from levels below. They do not represent the original pore fluid initially contained in the corresponding rock volume.

Thermal conv ection

Thermal convection arises from inverse density gradients. At increasing temperature, fluid density decreases and may reach a critical condition which defines the onset of thermal fluid migration. This critical condition is expressed by the Rayleigh number R. Thermal convection starts at Rayleigh numbers of R= 40 or values above.

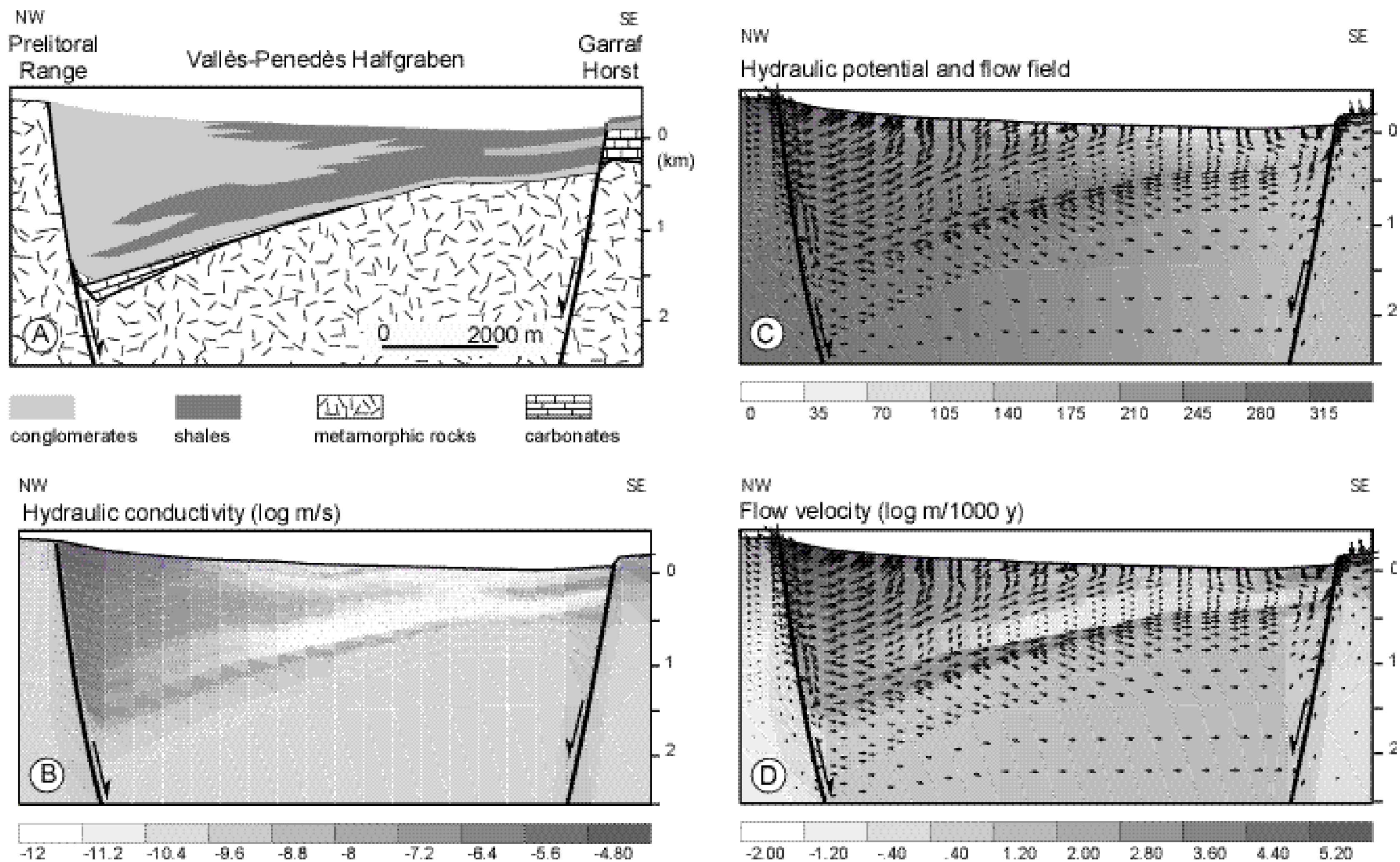
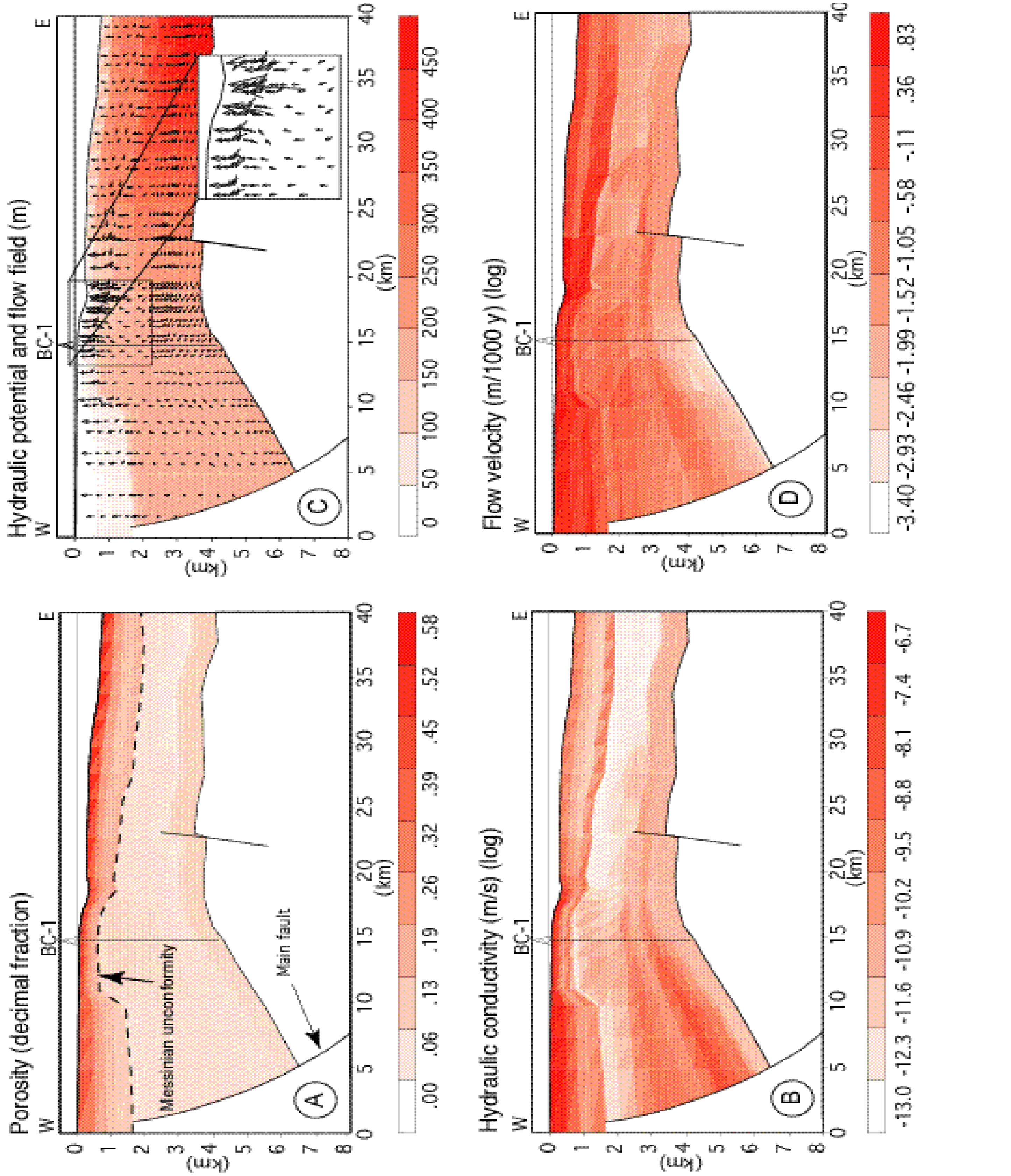


Figure 3. Topography driven fluid flow in the Penedès continental rift basin. Simplified geologic cross section (A). Hydraulic conductivity distribution (B). Calculated hydraulic potential and flow field (C). Calculated flow velocity and flow field (D).

Figura 3. Flujo controlado por la topografía en la cuenca de rifting continental del Penedès. Corte geológico simplificado (A). Distribución de la conductividad hidráulica (B). Potencial hidráulico y campo de flujo calculados (C). Velocidad de flujo y campo de flujo calculados (D).



Porosity (decimal fraction)
Hydraulic conductivity (m/s) (log)
Hydraulic potential and flow field (m)
Flow velocity (m/1000 y) (log)
W
E
BC-1
Messinian unconformity
Main fault
A
B
C
D
(km)
.00 .06 .13 .19 .26 .32 .39 .45 .52 .58
-13.0 -12.3 -11.6 -10.9 -10.2 -9.5 -8.8 -8.1 -7.4 -6.7
0 50 100 150 200 250 300 350 400 450
-3.40 -2.93 -2.46 -1.99 -1.52 -1.05 -.58 -.11 .36 .83

Thick and permeable layers allow more easily the onset of thermal convection. However, the heterogeneity of sedimentary basins tends to suppress the generation of large convection cells.

As solute concentrations increase with depth, the inverse density gradient from increased temperatures at depth is usually more than counteracted by the density increase from elevated solute concentrations with depth. A salinity increase in the order of 25 mg/l /km is sufficient to remove the reverse density gradient created by the thermal expansion of water (Bjørlykke et al., 1988). Convection due to high densities at shallow depth, for example around salt layers or salt domes, may also cause fluid flow; however, salinity stratification around salt domes in Louisiana shows that convection is very slow (Ranganathan and Hanor, 1988), and a density overturn does not take place for a long time. Convection cells do not develop if overpressure causes forced fluid flow which is stronger than the forces which drive thermal convection (Bjørlykke and Gran, 1994).

Thermal convection can drive fluid flow and transport of solutes, involving a circular flow pattern with rising fluids at elevated temperatures on one side of the convection cell and cooled fluids moving down on the other side. It is restricted to locations with elevated thermal gradients and sufficiently thick aquifers. It may produce important fluid rock interaction due to the elevated mass transport and rapidly changing physical and chemical conditions of the fluids along their paths. Mineralization around plutons is considered as a result of thermal convection around a cooling intrusion (Ferry and Gerdes, 1998). Such recent flow systems have been studied at the Wairakei (New Zealand) geothermal fields, which are caused by a shallow magmatic intrusion (Simmons et al., 1992). The observation of layerwise distribution of saline fluids in many sedimentary basins indicates that such circulation patterns are more likely to be local phenomena not operating at basin scale (Bjørlykke et al., 1988), even if the basin fill includes high permeable units. Elevated heat flow may occur during tectonic subsidence of sedimentary basins. As hydraulic gradients either from topography or from consolidation tend to inhibit thermal convection, such circulation patterns are restricted to situations, where consolidational or topography driven fluid flow can be neglected.

FLUID FLOW IN DIFFERENT BASIN SETTINGS

Sedimentary basins develop different flow systems depending on their structural setting. Three different types of basins are discussed here: continental rift basins with predominantly topography driven fluid flow, marine rift systems with consolidational fluid flow, and thrust systems with consolidational fluid expulsion due to thrusting.

Continental rift basins

Topography driven fluid flow commonly occurs in continental rift basins, which extend up to several hundreds of kilometers length and width of tens of kilometers. The hydraulic regime of such basins is largely controlled by their tectonic evolution and topographic configuration. As sedimentation in rift basins often starts with coarse grained material covering large parts of the evolving basin, such basins are likely to develop deep regional basal aquifers, capable of redistributing fluid, solutes and heat. Typically, topography-driven flow develops due to basin subsidence and uplift of its shoulders. The bounding normal faults and fracture zones and the more permeable sediments at the basin edges facilitate infiltration of meteoric fluids, while the finer and less permeable sediments in the central parts reduce flow rates. At later stages, parts of the basin may be controlled by lacustrine or marine conditions and topography driven flow is replaced by consolidation as the principal mechanism of fluid migration. When subsidence slows down and erosion of rift shoulders continues, topographic gradients decrease, and in the absence of topography driven flow, thermal driven convection cells may locally develop, especially in coarse and permeable units close to the bounding faults. Post-rift sediments may later cover syn-rift sediments, providing hydrogeologic systems governed by consolidational flow. Depending on sedimentation history, regional aquifers may develop during this stage which ad-

Figure 4. Consolidation-driven flow field in the simulated section of the Barcelona half-graben with well BC-1. Simplified cross section (A). Calculated hydraulic conductivity (B). Hydraulic potencial and flow field (C). Flow velocity (D).

Figura 4. Flujo por consolidación en la sección simulada del semigraben de Barcelona con indicación del sondeo BC-1. Corte geológico simplificado (A). Distribución de la conductividad hidráulica (B). Potencial hidráulico y campo de flujo (C). Velocidad de flujo (D).

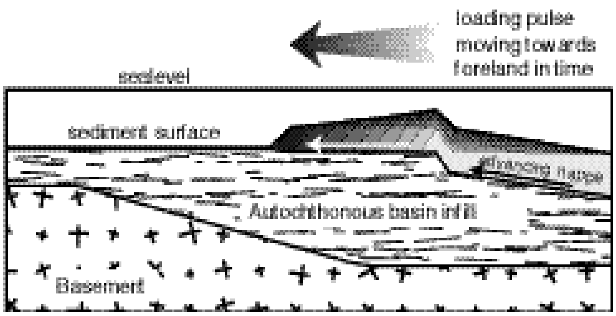


Figure 5. Emplacement of a moving thrust-sheet over an autochthonous foredeep sedimentary basin infill and related maximum loading zone moving with the thrust front.

Figura 5. Emplazamiento progresivo de un cabalgamiento sobre una cuenca sedimentaria autóctona mostrando la migración de la zona de carga máxima durante el movimiento del frente de cabalgamiento.

ditionally redistribute fluids. Rift basins are often strongly asymmetric with respect to their length axis, which is reflected in topography as well as in facies distribution. The more subsiding side is therefore likely to develop elevated hydraulic gradients. Depending on the configuration of the hydrostratigraphic units of a basin and its topographic elevation, fluid discharge may be located on the less subsiding part, providing geothermal anomalies as described for the Rhine-graben (Clauser, 1989).

Topography driven flow has been proposed by Travé et al. (1998) and Travé and Calvet (in press) to explain diagenetic processes taking place in the Vallès-Penedès half-graben, a continental rift basin in the Catalan Coastal Range (Fig. 2). Different evolutionary steps of the flow field during the neogene rifting process have been identified by Travé et al. (1998) based on geochemical and isotopical analyses of fracture cements and host rocks. Fluid flow through the basin fill has been simulated using a simplified cross section of the basin (Fig. 3a). The location of the simulated cross section presented here is shown on figure 2. The basin is asymmetric and bounded by normal faults. The thickness of the basin fill reaches up to 2,500 m of cenozoic sediments at its NW boundary and about 1,000 m at its SE boundary. The principal fluid recharge area is located in paleozoic to cenozoic rocks at the NW boundary at elevations up to 450 m. The Garraf horst with mesozoic carbonates forms the SE boundary and provides minor topography driven flow due to its lower topographic elevation. Fluid discharge is located in the central parts of the basin with low topographic elevation. The distribution of hydraulic conductivity (Fig 3b) has been extrapolated from the sediment facies and includes a permeable basal unit and several permeable units at the NW boundary of the basin formed by Burdigalian (lower Miocene) to Serravalian (middle Miocene) conglomerates. The central part of the basin is formed by less permeable units. A principal objective of the simulation model is to evaluate the influence of the bounding faults on the basin hydrology. The faults are incorporated as zones of elevated hydraulic conductivity. The resulting flow system (Fig. 3c) corresponding to upper Miocene time demonstrates meteoric fluid infiltration on the NW boundary into the deeper units constituted by basal conglomerates that act as a regional aquifer. Fluids from the NW boundary flow towards the SE boundary and ascend along the bounding fault. Calculated maximum flow velocities (Fig. 3d) are in the order of hundreds of m/y with maximum velocities close to the NW boundary due to elevated topographic gradients and high permeable conglomerates at shallow depth. Flow in the central parts of the simulated cross section is reduced due to the presence of low permeable shales. The basal conglomerates, which may represent a regional aquifer, develop maximum flow velocities in the order of several m/y. At the SE boundary, fluids from the opposite boundary mix with meteoric fluids from the Garraf horst. Such a flow system is responsible of upper Miocene dolomitization of siliciclastic rocks cropping out in this area (Calvet et al., in press).

Marine rift basins

If marine conditions prevail, consolidational fluid flow is the principal process in fluid flow and advective transport of solutes and energy. Such conditions occur in passive margin basins and associated rift basins. The Barcelona half-graben is presented here as an example of consolidational fluid flow. The simulated section has been adapted from Bartrina et al. (1992) (Fig. 2). Sedimentation in the Barcelona half-graben was mainly under marine conditions except for the lowermost units. The geometry of the basin is similar to the Vallès-Penedès half-graben that was formed in the same tectonic context. The Barcelona half-graben is asymmetric with up to 6 km thick sequence of cenozoic sediments at the NW boundary, represented by a listric fault (Fig. 4). Thickness of cenozoic sediments decrease to 3 km towards SE. Mesozoic carbonates represent the lowermost unit of the simulated section. Coarse grained sediments with elevated hydraulic conductivities are deposited close to the bounding fault, interfingered with fine-grained and less permeable

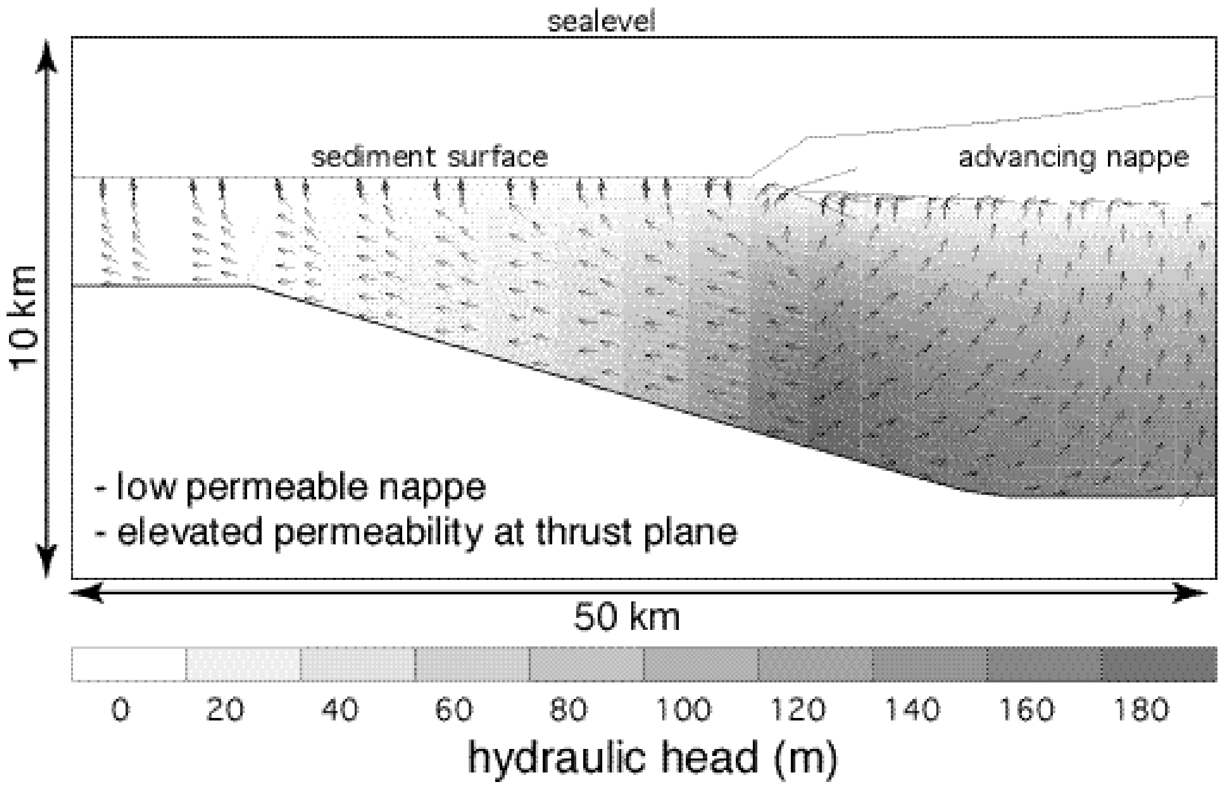


Figure 6. Simulated flow field and fluid pressure distribution due to a moving maximum loading zone at the thrust front.

Figura 6. Campo de flujo y distribución de la presión de fluido originada por el movimiento de la zona de carga máxima en el frente de cabalgamiento durante el emplazamiento de un manto.

deposits towards the SE. Upper Miocene deposits are entirely marine. An important feature of the cross section is the Messinian discontinuity between the upper Miocene and the Pliocene to Quaternary deposits (Fig. 4a). The Messinian discontinuity represents a sharp sea level fall in the Mediterranean Sea, allowing topography driven flow to occur in the basin. Pliocene to Quaternary deposits above the discontinuity reach thicknesses of up to 1,500 m and cause consolidational fluid flow. The compaction equilibrium is probably not yet reached in all parts of the basin. A paleohydrogeologic simulation of the basin has been performed in order to characterize fluid flow, overpressures and the thermal history during basin evolution (Bitzer, 1997). Figure 4 shows the assumed distribution of hydraulic parameters (Fig. 4b) and the simulated consolidational flow pattern for the present situation (Fig. 4c). The simulated flow field is characterized by two interacting systems. In the western side, the circulation pattern is dominated by consolidation induced fluid expulsion due to the elevated Pliocene to Quaternary sedimentation rates, resulting in a fluid flow towards east. On the eastern side of the simulated section, high sedimentation rates in conjunction with low permeable sediments lead to overpressures up to 400 m and to a fluid expulsion towards west. Both systems meet in the central part, where the Messinian paleo-relief is covered by Pliocene and Quaternary sediments with reduced thickness. The horst-like structure at well BC-1 represents therefore a hydraulic trap with elevated flow velocities (Fig. 4d). Heat advection is negligible due to the reduced flow rates. While some of the model assumptions are uncertain, the parameters used in the simulation model have shown to coincide with data derived from well logs (Negredo et al., 1994, Bitzer, 1997).

Thrust systems

Fluid flow in thrust systems may involve topography driven flow, if parts of the thrust are located above sea level. Consolidational driven flow may result from the load of the advancing nappes and to some degree from the lateral compression. Oliver (1986) proposed that fluids may be mobilised from thrusting, migrating over large distances along thrust planes as preferential pathways. He suggested that such fluids finally move into foreland basins where they may contribute to the formation of mineral resources. While this concept is appealing, modelling of fluid flow and heat transport in a thrust belt performed by Deming et al. (1990) demonstrated that flow velocities are in the order of centimetres per year and thermal anomalies in the order of 5ºC. This is insufficient to contribute to significant mass and energy transfer. Bethke and Marshak (1990) also state that fluid expulsion in convergent margins is far too low to produce efficient advective heat transport. The hypothesis of Oliver (1986) therefore requires complementary assumptions like extreme flow channelling and episodic dewatering. Such flow channelling along a basal regional aquifer and fast consolidational fluid expulsion from a fast moving thrust may cause slight changes (Deming et al., 1990, Bitzer et al., 1998), however thermal effects still remain orders of magnitude below those caused by topography driven flow.

Fluid flow during thrusting depends to a large extent on the velocity of the thrust and its hydraulic properties (Bitzer et al., 1998). As the thrust moves upon a non-moving block, fluid expulsion results from a continuously moving loading zone represented by the thrust front. This point of maximum loading (Fig. 5) controls the consolidational fluid expulsion. Assuming that the thrust has a homogeneous thickness, the loading pulse is located at the thrust front, i.e. the position of the thrust front represents the location of maximum loading. The resulting flow field and pressure distribution depends strongly on the existence of preferential pathways, the permeability of the nappe and basin heterogeneity (Bitzer et al., 1996). In the example given here, the thrust zone is assumed to be a preferential pathway, which drains fluids expelled during thrust emplacement. As a result, maximum consolidational pressure is located below the thrust front. Fluid flow is directed into the reverse direction of thrust movement in some portions of the overthrusted basin (Fig. 6). In case the thrust plane does not represent a preferential pathway, overpressures accumulate from previous stages of thrusting, and maximum overpressures are located in the previously overthrusted parts of the basin (Bitzer et al., 1998).

SHORT TERMED FLOW EVENTS

Fluid flow in sedimentary basins is not necessarily always a continuous and steady process. Short termed episodic fluid flow events along preferential pathways such as faults or fracture zones are increasingly being studied as efficient processes in the generation of mineral deposits. Effects of episodic dewatering and seismicity induced fluid flow are presented here.

Episodic dew atering

Hydrofractures in rocks indicate temporal existence of fluid overpressures capable of causing ruptural deformation at a given stress regime (Wang and Xie, 1998; Sibson, 1981). A possible source of such overpressures is sediment consolidation. However, hydrofracturing has been observed at shallow depth, where consolidation derived overpressures would not be expected from the hydraulic properties of sediments at shallow depth. An episodic fluid release from a deep-seated source might account for temporarily elevated fluid pressures at shallower depth. Such a process might be initiated by a spontaneous opening of a fault or fracture zone with elevated hydraulic conductivity, connecting an overpressured compartment at depth with a low pressure hydrostratigraphic unit at shallower depth (Fig. 7). A rapid fluid expulsion would have several effects: a) it could locally and temporarily create a pronounced thermal disequilibrium between fluid and rock; b) it could move fluids into a geochemically different environment; c) it might involve mixing of different fluids; d) it would cause a pressure drop within the overpressured compartment at depth and e) it will create a pressure increase in the overlying units. These units could suffer hydrofracturing due to increased fluid pressure and because of reduced $\sigma 3$ (lithostatic load)

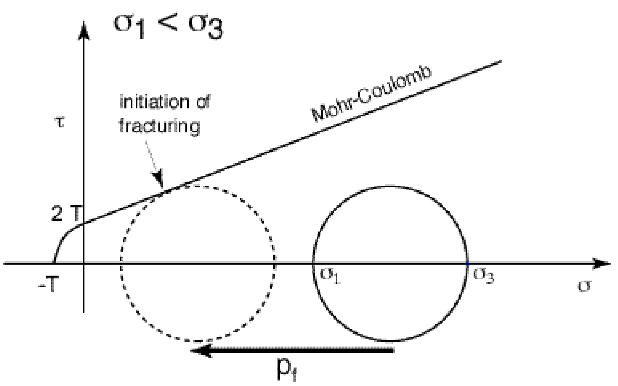


Figure 7. Increase of fluid pressure (pf) necessary to create rock failure.

Figura 7. Incremento de la presión de fluido (pf) necesario para fracturar la roca.

at shallower depth (Phillips, 1972). A moderate increase in fluid pressure can therefore be sufficient to initiate hydrofracturing at shallow depth.

The assumption of chemical equilibrium between porewater and rock in sedimentary basins is in most cases justified due to low flow rates. However, it might be strongly disturbed when episodic dewatering is involved and flow velocities are high in comparison to reaction rates. Mineral precipitation within hydrofractures takes place from fluids which cause fracturing. This is facilitated by the fact that minerals will tend to precipitate in the fracture as they are only subject to pore pressure, whereas the same mineral in the rock matrix may have a tendency to dissolve due to tectonic stresses. Ascending cooling pore fluids may cause precipitation of quartz and dissolution of calcite as silicates have low solubilities at low temperatures, whereas carbonates show retrograde solubility. As fluid pressure in the fracture decreases, a degassing of carbon dioxide may further facilitate carbonate precipitation.

Episodic fluid flow has been considered by Cathles and Smith (1983) as a possible process involved in the generation of MVT lead-zinc mineralizations in North America. Due to the reduced transport capacity of this fluid moving process, it is assumed that episodic dewatering must occur repeatedly to account for the extent of the observed mineralizations. The model of episodic dewatering avoids the problem pointed out by Deming and Nunn (1991) that elevated heat flow from topography driven advection is incompatible with the presence of mineralizing brines. However, as stated before, consolidation implies a closed flow system without recharge, and therefore fluid and solute mass involved in episodic dewatering is limited in its quantity.

A numerical experiment demonstrates the effect of episodic dewatering and its capacity to transport solutes. A sedimentary sequence with four hydrostratigraphic units is defined (Fig. 8) with an overpressured basal unit with hydraulic conductivities in the order of 10-7 m/s. Overpressure is defined through the ratio between fluid pressure and total load (λ) which is set to 0.65 in the experiment. The value of λ at hydrostatic conditions at shallow depth is in the order of 0.4. Overlying unit 2 represents a low permeable seal and separates unit 1 from a permeable layer at shallow depth, unit 3. Finally, unit 4 is low permeable and defined by hydrostatic conditions at its upper boundary. It is as-

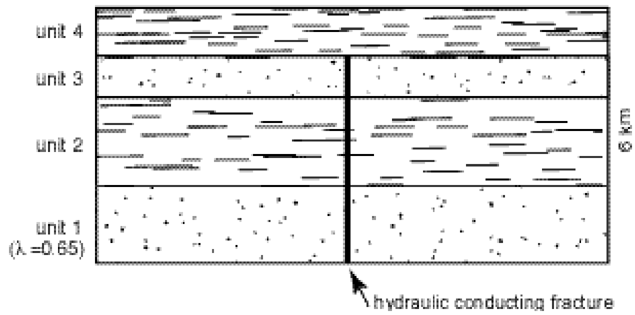


Figure 8. Hydrostratigraphic units for experiment involving episodic dewatering of an overpressured compartment.

Figura 8. Unidades hidroestratigráficas consideradas en el experimento de pérdida episódica de fluidos de un compartimento sometido a sobrepresión.

sumed that at t=0 a vertical fracture zone opens a hydraulic connection between the overpressured basal unit and the aquifer represented by unit 3. As the model is symmetrical with respect to the vertical fracture zone, it is sufficient to simulate a halfspace and to situate the fracture zone at a boundary of the model.

Figure 9 shows the evolution of the flow field at different stages of the dewatering process. The fracture zone is located at the left boundary. Fluids start immediately after opening of the fracture zone to be drained from the overpressured unit 1 towards unit 3. Synchronously, fluid pressures decrease in unit 1 and increase in unit 3. After 21,000 years fluid pressure in unit 1 has decreased to about half of its initial value. Dewatering of unit 1 and invasion of fluids in unit 3 continue.

In order to show the capacity for solute transport, a conservative tracer is placed in unit 1. Figure 10 shows the evolution of solute concentration in response to advective transport. After 21,000 y solutes haven been migrated into unit 3, and as dewatering is not finished yet, solutes will continue to move further. The example demonstrates that episodic dewatering from an overpressured compartment may create considerable fluid and solute transport, if the flow system provides sufficient consolidational released fluids and if the flow event is sufficiently long termed.

This experimental configuration might be applied to natural rift basins, with unit 1 presenting permeable early syn-rift sediments, unit 2 less permeable late syn-rift sediments, and units 3 and 4 permeable post-rift sediments which create some overpressure due to consolidation in

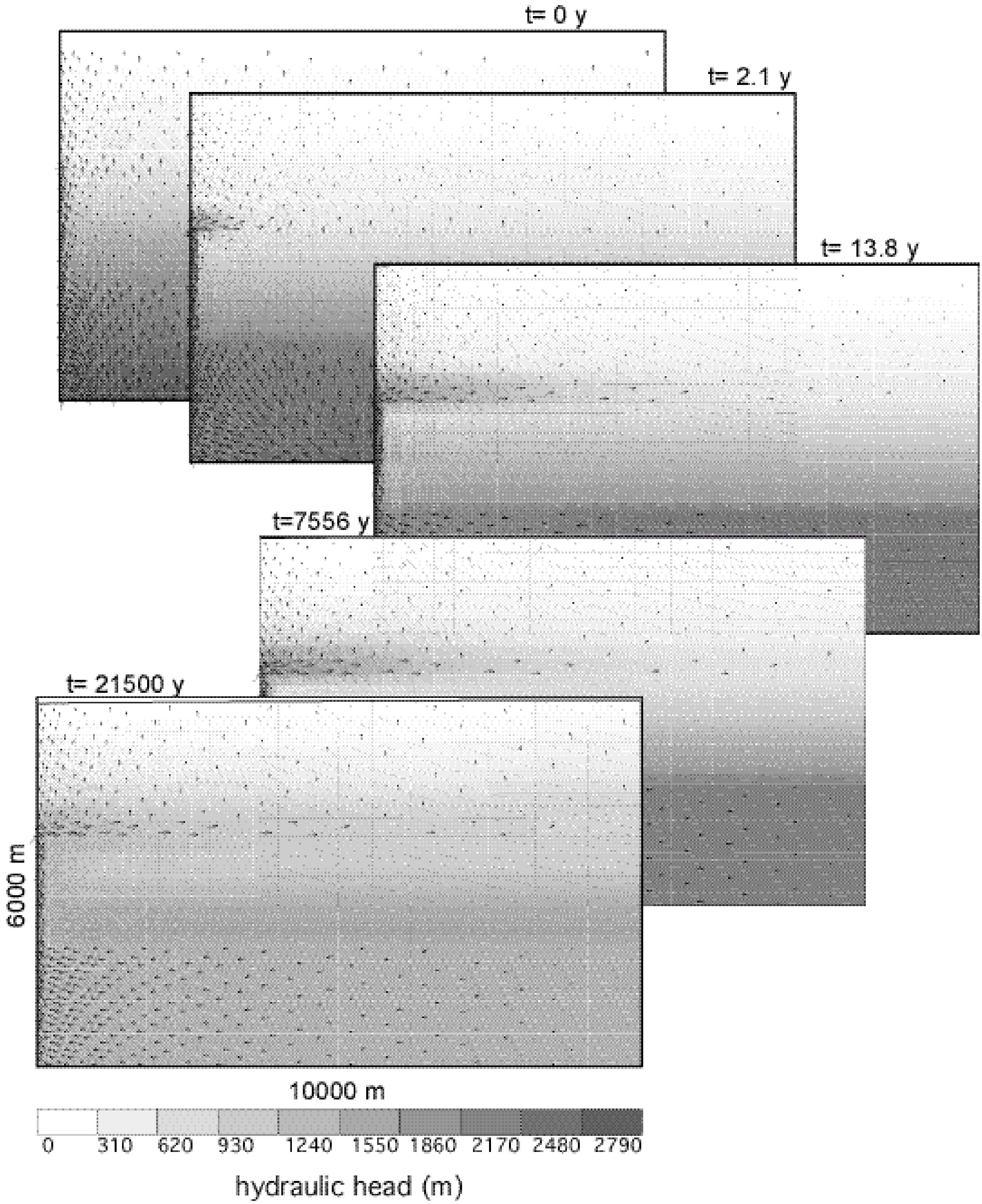


Figure 9. Evolution of fluid pressure and flow field after connecting an overpressured compartment with a shallow aquifer.

Figura 9. Evolución de la presión de fluidos y del campo de flujo, después de conectar un compartimento sometido a sobrepresión con un acuífero superficial.

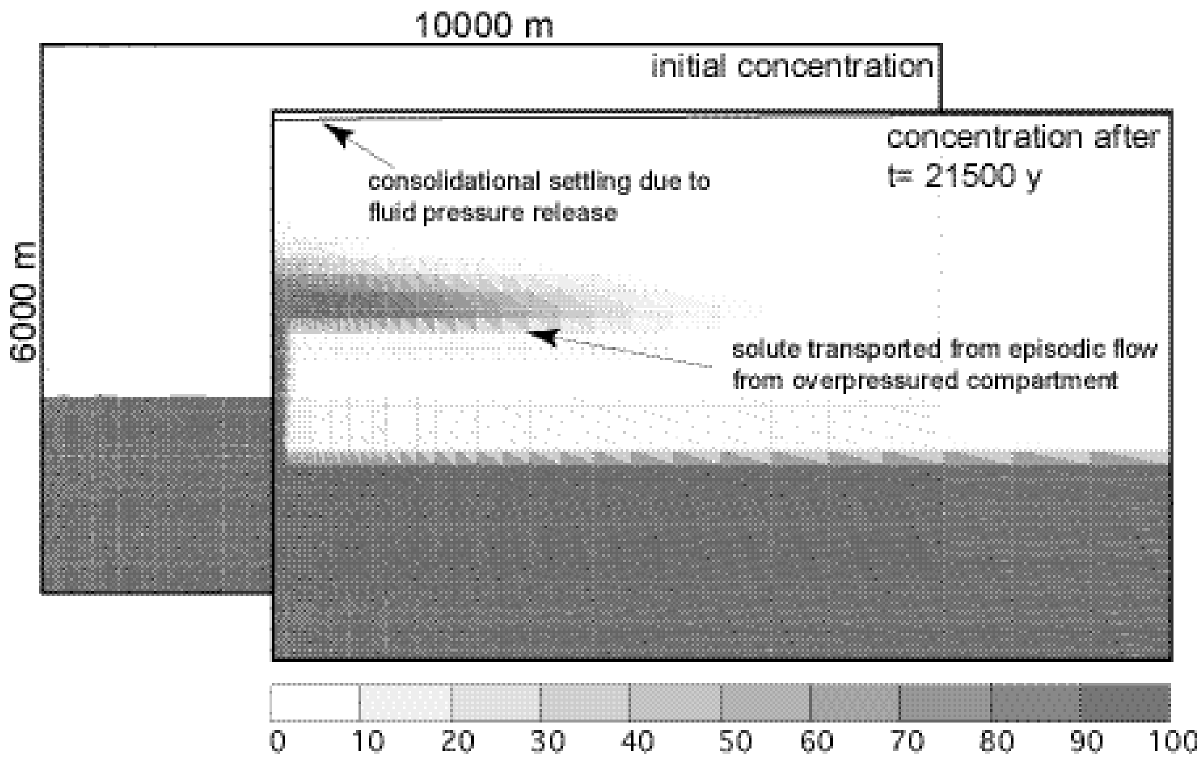


Figure 10. Transport evolution of a conservative tracer due to episodic fluid release from an overpressured compartment.

Figura 10. Evolución del transporte de un trazador conservativo desde un compartimento sometido a sobrepresión en el que se produce una pérdida episódica de fluido.

the units below. The bounding fault zone may occasionally be reactivated, thereby draining overpressured fluids from lower units and contributing to mineralization in the rift-bounding faults and post-rift sediments.

Seismicity induced f low

Fluid migration may also be related to pore fluid expulsion during seismic shocks. The hydrologic response to these processes is often observed in the aftermath of earthquakes as changes in river discharge and in hydraulic head. These hydraulic effects often take place over days and weeks. Muir-Wood and King (1993) showed that the hydraulic response to earthquakes depends strongly on the tectonic setting. Whereas earthquakes in distensive settings often show rising heads and increased discharge, compressive settings show less pronounced effects and occasional lowering in heads and decrease of river discharge. Muir-Wood and King (1993) assumed that, in distensive settings, pore space is created due to accumulation of shear stress in rocks prior to the earthquake. During the subsequent earthquake pore space collapses and fluids are expulsed towards the land surface along the more conductive zones of the affected rock body or along fault zones. Some authors (Rojstaczer and Wolf, 1992) suggest an increase in hydraulic conductivity due to creation of new fractures as the cause for such changes, however the detailed study of hydraulic response in compressive and distensive settings by Muir-Wood and King (1993) underlines the predominance of the coseismic strain process.

CONCLUDING REMARKS

Different flow systems contribute to the transfer of fluids, solutes and heat in sedimentary basins. Topography driven flow operates from a local to a regional scale and provides high flow velocities with a significant capacity to transport solutes and heat in sedimentary basins. Topography driven flow predominates in continental rift basins and basins which have been subaerally exposed during tectonic inversion. Consolidation driven flow is caused by loading of compressible sediments and results in an expulsion of interstitial pore fluids. In contrast to topography driven flow, consolidational flow is limited by the absence of a recharge process. Flow velocities are in general several orders of magnitude below topography driven flow, however consolidation is the principal fluid moving process in all submarine sedimentary basins. Flow velocities originated by consolidation are lower than or similar to the sedimentation rate. Important effects of consolidation are the occurrence of fluid overpressures in low permeable sediments at high sedimentation rates and the change of hydraulic properties due to the reduction of pore space. Although the capacity for transport of solutes and thermal energy is comparably low, the vertical displacement of pore fluids in the growing sedimentary column has important implications on solute transport. Effects on heat flow are negligible. In case that episodic dewatering from an overpressured compartments occurs, flow velocities and transport capacity may be locally enhanced for a limited period of time and contribute to the generation of local mineralisation along fractured zones. Thermal convection may generate elevated flow rates, however it is probably not a process that operates at a basin scale. This is primarily due to the compensation of thermal related density contrasts from increasing solute concentrations with depth, the existence of topography or consolidation related hydraulic gradients and the heterogeneity of sedimentary deposits, which prevent the build up of large convection cells.

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APPENDIX

Equations for fluid flow, porosity dependent hydraulic conductivity and sediment compressibility and solute transport.

The transient flow equation (1) with $k_{x(\varphi)}$= porosity dependent hydraulic conductivity in x-direction using eq. (3.2.2), $\alpha_{(\varphi)}$= porosity dependent sediment compressibility, h= hydraulic head and φ=porosity (deMarsily, 1986) is solved for specified initial and boundary conditions.

$$(\delta/\delta x)(k_{x(\varphi)}+ \frac{\delta h}{\delta x})+(\delta/\delta z)(k_{z(\varphi)} \frac{\delta h}{\delta z})=(1-\varphi)\, \rho \mathbf{g} \alpha_{(\varphi)} \delta h/\delta t \quad (1)$$

The initial conditions in the model domain are defined through hydrostatic pressure. In the episodic fluid flow model, a depth-dependent overpressure is defined as initial condition in the entire model domain (2):

$$h_{t=0} = (p_h - \rho \mathbf{gz}) + p_{f(z)} \quad (2)$$

Consolidation is calculated assuming that total stress is transformed into effective stress acting between the sediment grains, and fluid pressure following Terzaghi´s principle (3):

$$\sigma_{load} = \sigma_{effective} + p_{fluid} \quad (3)$$

As fluids are drained, the effective stress increases and fluid pressure is released at the same rate (eq. 4):

$$\delta\sigma_{effective} + \sigma p_{fluid} = 0 \quad (4)$$

The equation of state for porosity expresses changes of porosity as a function of the solid portion of the sediment, fluid pressure change and porosity dependent sediment compressibilty $\alpha_{(\varphi)}$ (eq. 5):

$$\delta\varphi/\delta t = (1-\varphi)\alpha_{(\varphi)}\, \delta p_{fluid}/\delta t \quad (5)$$

and rearranging eq. 5 gives

$$\delta\varphi/\delta p_{fluid} = (1-\varphi)\, \alpha_{(\varphi)} \quad (6)$$

In order to express changes in hydraulic conductivity as a function of porosity the Kozeny-Carman relation is used (eq. 7) with S0= specific surface, μ = viscosity, ρw= density of pore fluid:

$$k = (\rho_w g \,/\, 5S_0^2 \boldsymbol{\mu})\, (\varphi^3 \,/\, (1-\varphi)^2) \quad (7)$$

As hydraulic diffusivity is presumably constant during compaction (Bredehoeft and Hanshaw, 1968) a similar function as the Kozeny-Carman equation for hydraulic conductivity with c=constant can be used for sediment compressibility (eq. 8):

$$\alpha = c\, (\varphi^3/(1-\varphi)^2) \quad (8)$$

Solute transport is calculated including diffusive, dispersive and advective transport and adsorption (eq. 9 with D= coefficient of molecular diffusion, Rf= retardation factor, ω= tortuosity, C= solute concentration, Dx, Dz = coefficient of hydrodynamic dispersion in x- and z-direction, vx, vz= flow velocities in x- and z-direction):

$$\begin{aligned} &D/(R_f\, \omega)\, ((\delta^2C/\delta x^2) + (\delta^2C/\delta z^2)) \\ &+ (D_x(\delta^2C/\delta x^2) + D_z(\delta^2C/\delta z^2))/R_f \\ &- (v_x(\delta C/\delta x) + v_z\, (\delta C/\delta z))/Rf \\ &= \delta C/\delta t \end{aligned} \quad (9)$$